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16. ABSTRACT

Our research is motivated by the need to protect the human chain and the environment from contamination by agricultural and industrial toxic chemicals. The objective of our research is to learn what plant mechanisms determine uptake, translocation, accumulation, and biodegradation of toxic chemicals in terrestrial plants. We believe that with this knowledge, a model can be developed that will be useful in understanding and predicting chemical fate in plants. We are also concerned about the effects of chemicals on the plants physiology and the resultant effect on uptake patterns and biomass production. Our work has been divided into the following three areas: database development, chemical fate experiments in plants, and model development.

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EPA/600/D-89/201

Research on fate and effects of toxic chemicals in terrestrial plants at EPA Corvallis Environmental Research Laboratory

by

Craig Mc Farlane

Our research is motivated by the need to protect the human food chain and the environment from contamination by agricultural and industrial toxic chemicals. Pesticides are mostly applied in conjunction with food production and have been formulated and regulated to minimize residues in harvestable produce. Industrial toxics are not regulated by the same philosophy and also pose a threat to food and environmental contamination from allowed or accidental release. In both cases, knowledge of possible routes of plant contamination and the reactions of organic chemicals in plants is needed to regulate chemical production and use.

The objective of our research is to learn what plant mechanisms determine uptake, translocation, accumulation, and biodegradation of toxic chemicals in terrestrial plants. We believe that with this knowledge, a model can be developed that will be useful in understanding and predicting chemical fate in plants. We are also concerned about the effects of chemicals on the plants physiology and the resultant effect on uptake patterns and biomass production. Our work has been divided into the following three areas: database development, chemical fate experiments in plants, and model

development.

DATABASES

In cooperation with Dr. John Fletcher of the University of Oklahoma we have developed the databases **PHYTOTOX** and **UTAB**. These databases are unique in the sense that they contain dose-response data. The numerical data have been taken from the published literature (1928-1988) and each response constitutes a record which is identified by the appropriate citation. The publication of these data in numerous journals over a 45 year period has made the data virtually inaccessible for daily routine work, since it is time consuming to recover the data from conventional library sources. Prior to the development of PHYTOTOX and UTAB the only efforts which had been made to organize these data were review articles and bibliographic listings, neither of which permitted direct access to data. As a result, only small portions of the total published data could be used at any one time, and the true value of this literature was not realized.

PHYTOTOX contains information about chemical toxicity to terrestrial vascular plants. Both natural and synthetic organic compounds administered to native, crop, or weed species have been considered. Information can be retreived by selecting data in combinations which may include: chemical (by name or CAS number), site and mode of chemical application, plant species, and the nature and magnitude of various responses. The database does not contain information pertaining to algae, fungi, inorganic

compounds, chemical mixtures, indirect effects, sequential applications, or physical-chemical properties. Phytotox is commercially available on-line through Chemical Information Systems as well as on a personal computer format using DBase III+.

UTAB is organized after the pattern of PHYTOTOX but contains information about the **U**ptake, **T**ranslocation, **A**ccumulation, and **B**iodegradation of organic chemicals in terrestrial plants. It presently exists only on the computer at the University of Oklahoma and is less developed and therefore less used than PHYTOTOX. Since this information is of increasing interest to persons doing risk assessment and toxic waste site clean-up and management, we intend to put more effort into cataloging UTAB data and will make it available in a personal computer format within the next two years.

The size of these databases is outlined below:

Database	Papers read	Records	Chemicals	Species
PHYTOTOX	4975	97,840	8602	2057
UTAB	1493	42,896	~1000	~350

Articles about the databases:

Fletcher, J.S., and F.L. Johnson. 1987. PHYTOTOX User's Manual. EPA Corvallis Environmental Research Laboratory, Corvallis OR

97333. c/o Craig Mc Farlane.

Fletcher, J.S., F.L. Johnson, and C. Mc Farlane. 1988. The influence of greenhouse versus field testing and taxonomic differences on plant sensitivity to chemical treatment. Environ. Tox. and Chem. (in press).

Fletcher, J.S., F.L. Johnson and J.C. Mc Farlane. 1988. Phytotoxicity data published on vascular plants. Environ. Tox. and Chem. (in press).

Fletcher, J.S., M.J. Muhitch, D. Vann, J.C. Mc Farlane and F. Benenati. 1985. PHYTOTOX database evaluation of surrogate plant species recommended by the U.S. Environmental Protection Agency and the Organization for Economic Cooperation and Development. Environ. Tox. and Chem. 4:523-532.

Fletcher, J.S. 1986. Development and use of PHYTOTOX and UTAB databases. Final project report (CR-807391-02-0 and CR-81195-02-0).

CHEMICAL FATE EXPERIMENTS

Our experimental work has involved determining the uptake patterns of several organic chemicals by plant roots and the subsequent fate of the chemical in plants. To accomplish this we needed a facility in which we could contain the toxic chemicals and assure that the plants were functioning normally. The facility constructed is a unique, computer-operated plant exposure/physiology laboratory. It provides numerous chambers, each providing two containments: one for the roots in either soil or hydroponic solution, and an aerial environment for the shoots. The two compartments are connected only by the stem. Environmental parameters are computer controlled and measured as are the photosynthetic, transpiration, and respiration rates of the test plants.

Experiments have revealed the following information:

- Root concentration is not proportional to uptake and translocation throughout plants.
- The chemicals studied (a series of substituted benzenes, and selected herbicides) are passively absorbed.
- Uptake differs from very rapid to non-detectable.
- Uptake of some chemicals is directly proportional to the rate of water flux.
- Many chemicals pass through the plants and are volatilized into the atmosphere.

- o In a series of experiments with nitrobenzene, using 8 species, the uptake and distribution could be described in proportion to water flux. However, the effects (sub-lethal and lethal) and metabolisms differed by species.
- o Accumulation (bio-concentration) is not necessary to account for phytotoxicity, nor to account for toxic levels (mammalian toxicity) of chemicals in plants.
- o Seeds and fruits are generally less susceptible to contamination via translocation from the roots due to the lower transpiration demands of these organs.

Articles on experimental studies:

Mc Farlane, C., T. Pfleeger. 1987. Plant exposure chambers for study of toxic chemical/plant interactions. J. Environ. Qual. 16(4):361-371.

Mc Farlane, C., C. Nolt, C. Wickliff, T. Pfleeger, R. Shimabuku and M. McDowell. 1987. The uptake, distribution and metabolism of four organic chemicals by soybean plants and barley roots. Environ. Tox. and Chem. 6:847-856.

Mc Farlane, C., T. Pfleeger, and J. Fletcher. 1987. Transpiration effect on the uptake and distribution of bromacil, nitrobenzene, and phenol in soybean plants. J. Environ. Qual. 16(4):372-376.

McCrady, J.K., C. Mc Farlane and F.T. Lindstrom. 1987. The transport and affinity of substituted benzenes in soybean stems. J. Exp. Bot. 38(196):1875-1890.

MODEL DEVELOPMENT

A mechanistic mathematical model (UTAB model) of a plant was constructed to describe **U**ptake, **T**ranslocation, **A**ccumulation, and **B**iodegradation of organic chemicals. It consists of one root, three stem and three leaf compartments, with each containing xylem, phloem, and storage. In one version, water flux is described by the water potential gradient from the soil solution (or hydroponic solution), through the plant to the atmosphere. Chemical movement is described by root binding, reflection at the endodermis, mass flow in the xylem and phloem sap, diffusion within each compartment, sorption to the materials of the compartments, and first order loss (metabolism or physical loss) from each compartment. The model uses the K_{ow}, diffusion coefficient, solubility and a derived reflection coefficient of the chemical.

The UTAB model has been successfully used to describe the influence of transpiration on the uptake and distribution of bromacil in soybeans. Additional validations are currently underway.

Articles describing the UTAB model:

Boersma, L., C. Mc Farlane, and T. Lindstrom. 1988. Uptake and transport of chemicals by plants. Three leaf model. (Version 2.1) Users Guide. Oregon State Univ. Dept. of Soil Science, Corvallis OR.

Boersma, L., T. Lindstrom, C. Mc Farlane and E.L. McCoy. 1988. Uptake of organic chemicals by plants: A theoretical model. Soil Sci. (in press).

Boersma, L., F.T. Lindstrom, C. Mc Farlane, E.L. McCoy. 1988. Model of coupled transport of water and solutes in plants. Special Report 818. April 1988. Agricultural Experiment Station, Oregon State University, Corvallis OR.

Lindstrom, F.T., L. Boersma, C. Mc Farlane, K.P. Suen, D. Cawlfield. 1988. Uptake and transport of chemicals by plants (Version 2.1) Special Report 819. May 1988. Agricultural Experiment Station, Oregon State University. Corvallis, OR.

Lindstrom, F.T., L. Boersma, C. Mc Farlane. 1987. Steady state fluid transport model for plants. In Larry G. James and Marshall J. English (eds) Irrigation Systems for the 21st Century pp. 568-575. American Society of Civil Engineers, New York.

Link, S.O., R.J. Fellows, D.A. Cataldo, J.G. Droppo, and P. Van Voris. 1987. Estimation of aerial deposition and foliar uptake of xenobiotics: Assessment of current models. Pacific Northwest Laboratory PNL-6173/UC-11 (C. Mc Farlane Project officer).